Ethyl 1-naphthaleneacetate

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.78

Global applicability domain: Inside

Local applicability domain index: 6.75e-01

Confidence level: 6.85e-01

Nearest Neighbors from the Training Set

Image not found
Clofibric acid
Measured: 2.57
Predicted: 2.83

Image not found
2,3-Dimethyl-4H-chromen-4-one
Measured: 2.31
Predicted: 2.68

Image not found
Alclofenac
Measured: 2.48
Predicted: 2.61

Image not found
Mecoprop
Measured: 3.13
Predicted: 2.43